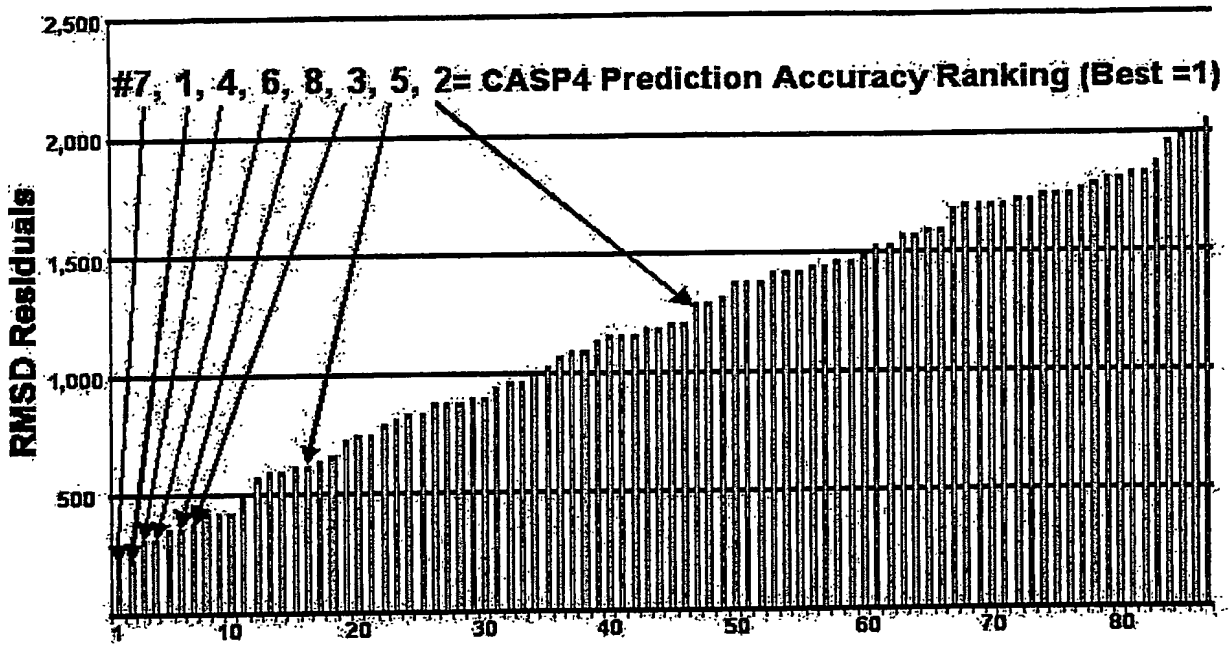

Figure 1

BEST AVAILABLE COPY

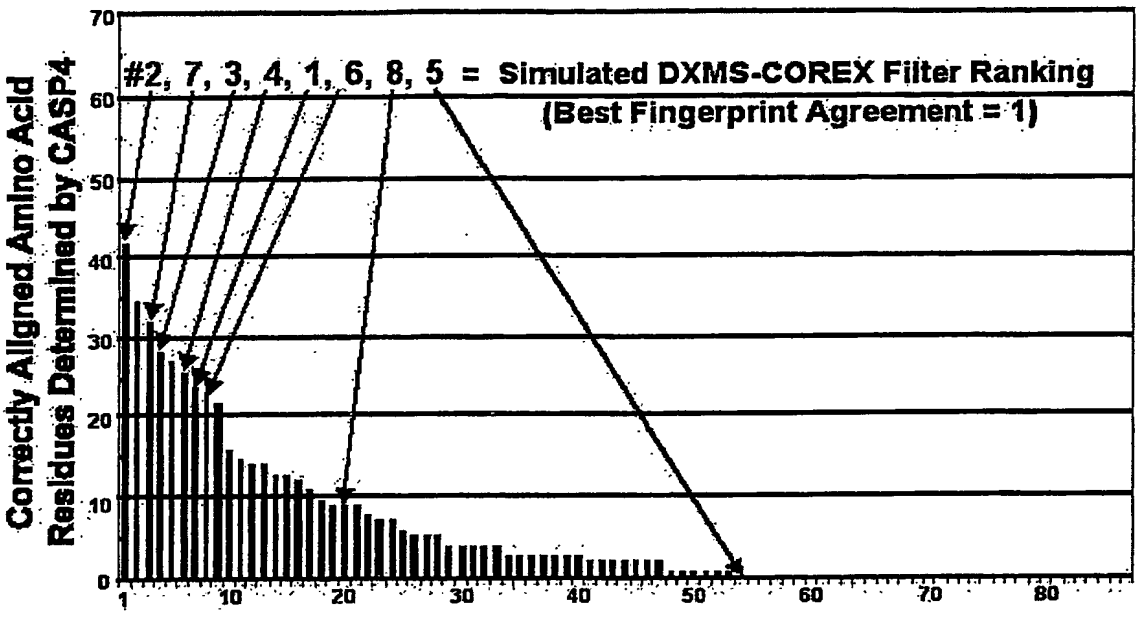
#2, 7, 3, 4, 1, 6, 8, 5 = Simulated DXMS-COREX Filter Ranking
(Best Fingerprint Agreement = 1)
Correctly Aligned Amino Acid Residues Determined by CASP4
70
60
50
40
30
20
10
0
1
10
20
30
40
50
60
70
80

Figure 2

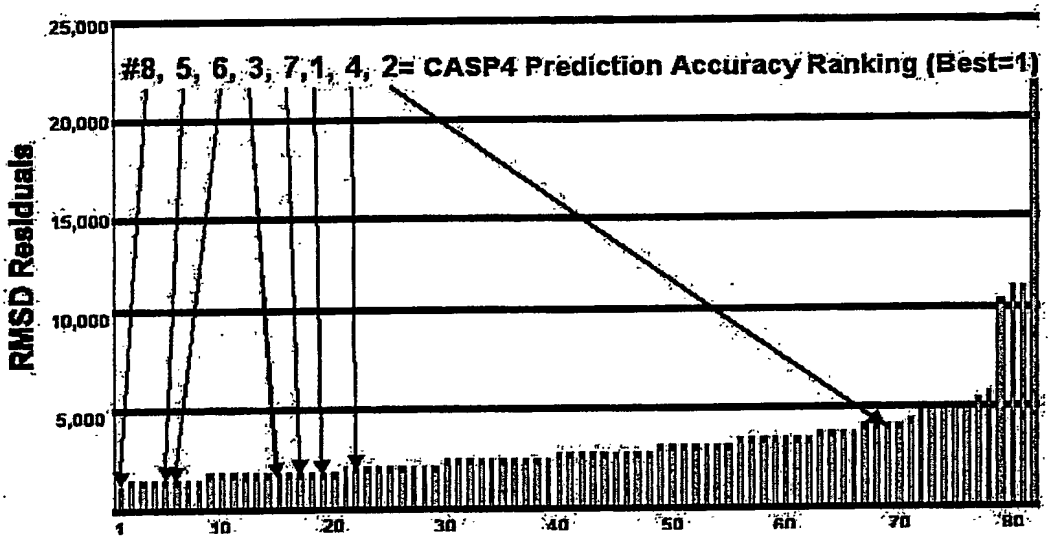
#8, 5, 6, 3, 7, 1, 4, 2= CASP4 Prediction Accuracy Ranking (Best=1)
RMSD Residuals
25,000
20,000
15,000
10,000
5,000
1
10
20
30
40
50
60
70
80

Figure 3

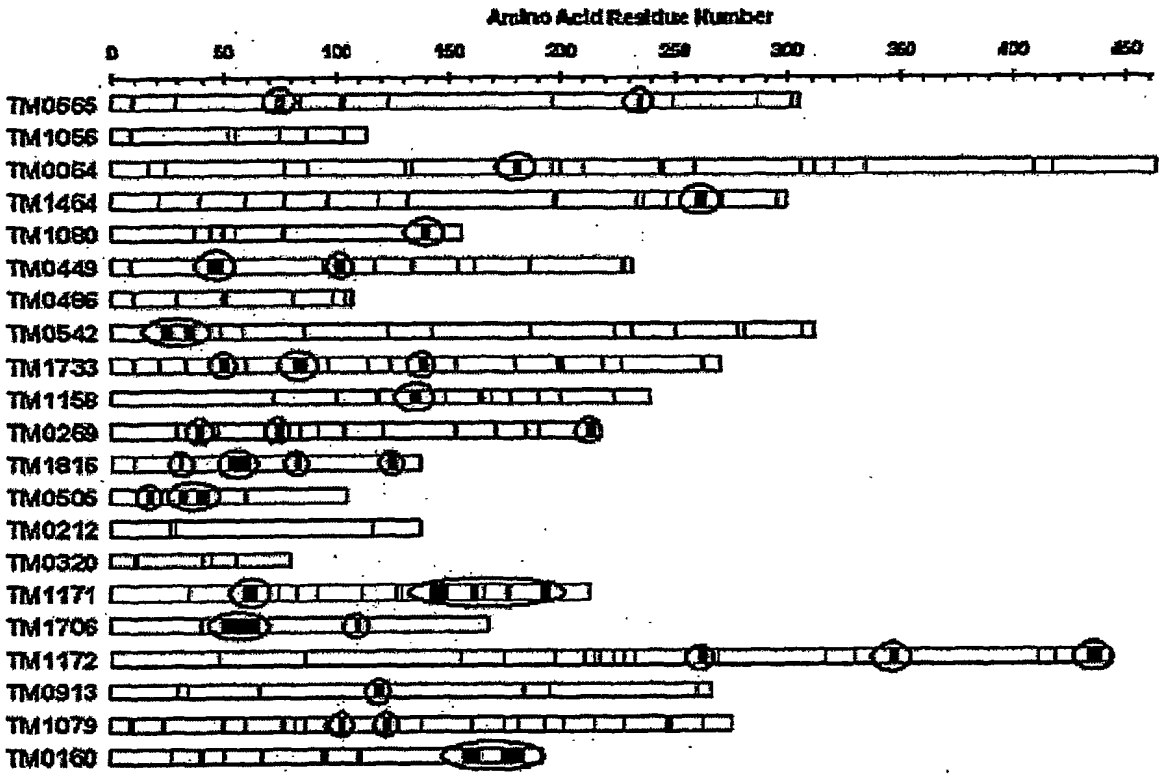
Amino Acid Residue Number
0
50
100
150
200
250
300
350
400
450
TM0565
TM1056
TM0064
TM1464
TM1080
TM0449
TM0496
TM0542
TM1733
TM1158
TM0269
TM1815
TM0505
TM0212
TM0320
TM1171
TM1706
TM1172
TM0913
TM1079
TM0160

Figure 4

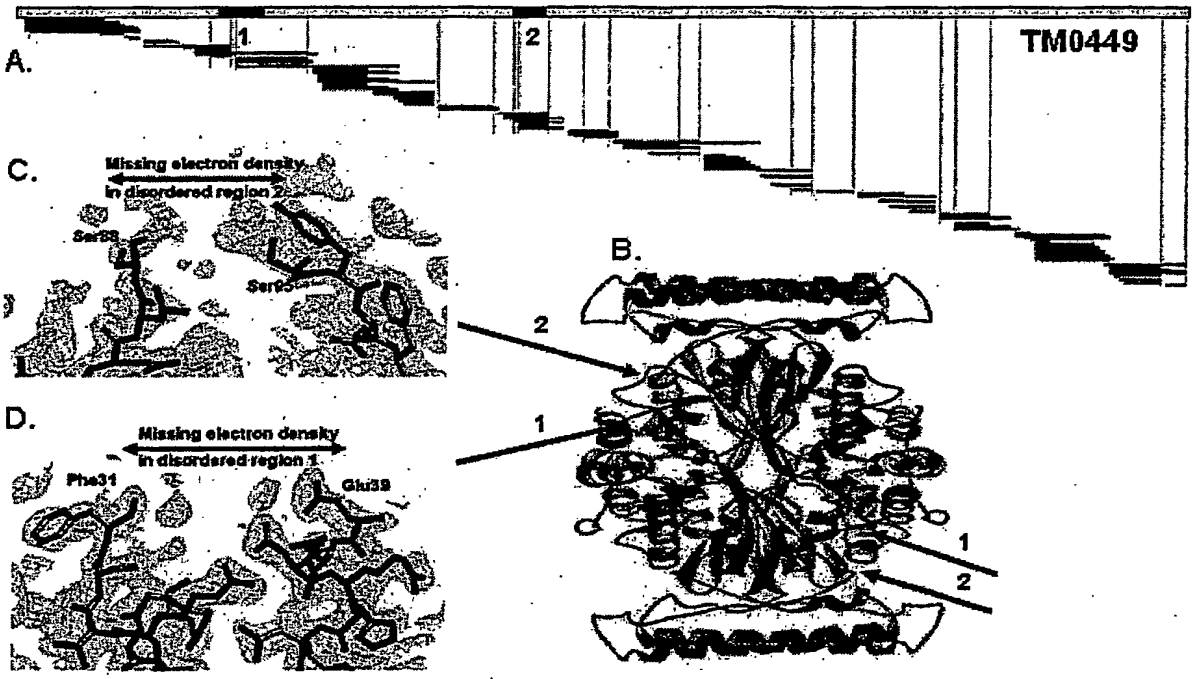
A.
1
2
TM0449
C.
Missing electron density
in disordered region 2
Ser28
Ser35
B.
2
1
D.
Missing electron density
in disordered region 1
Phe31
Glu39
1
2

Figure 5

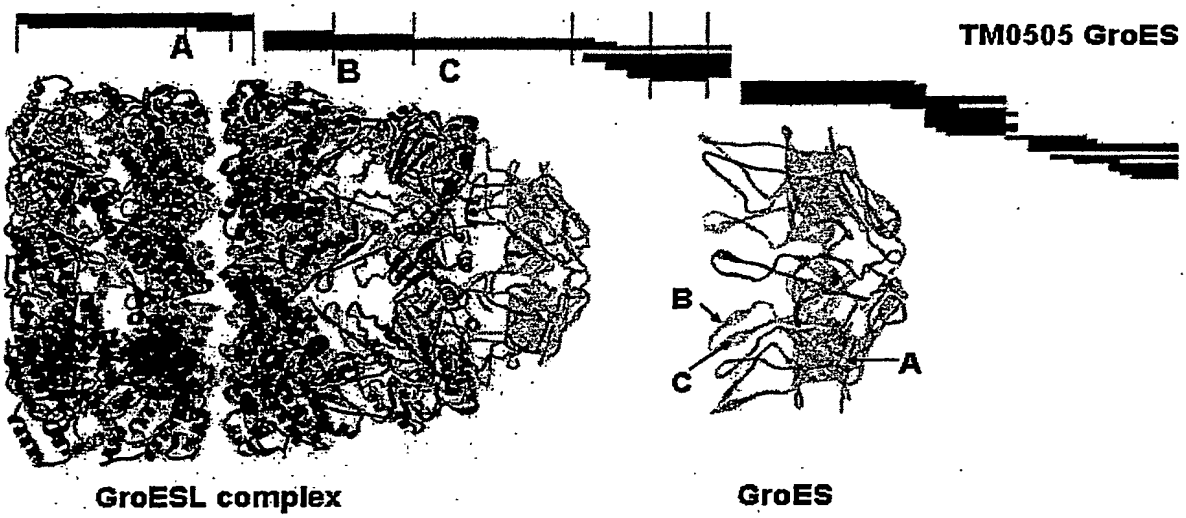

Figure 6

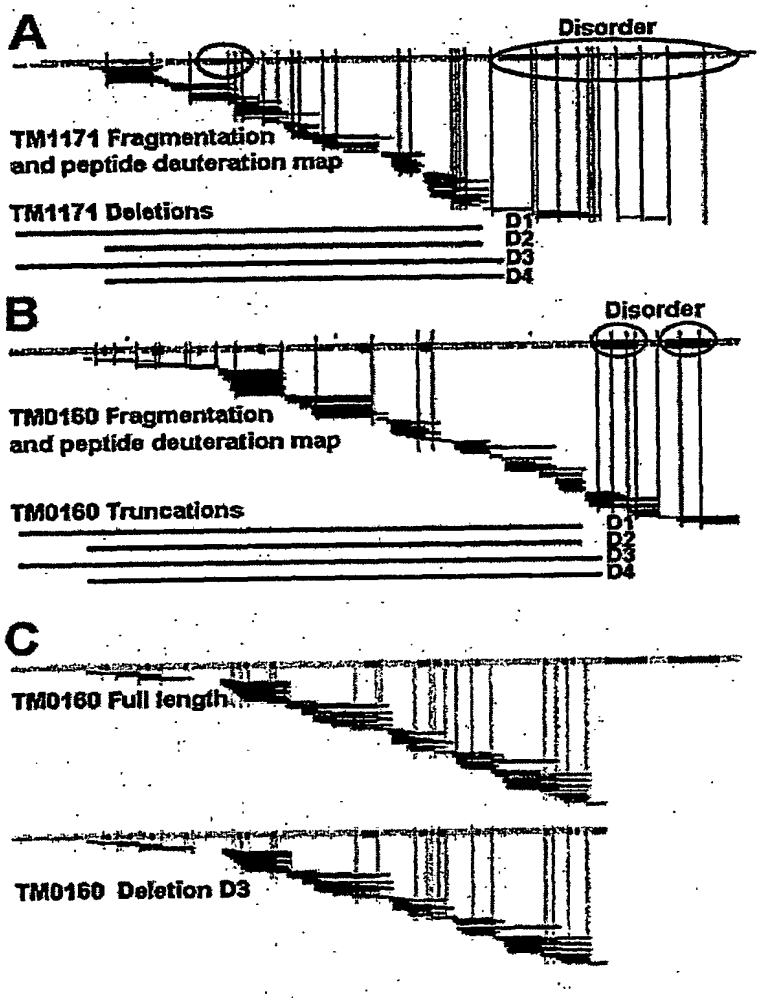
A
Disorder
TM1171 Fragmentation
and peptide deuteration map
TM1171 Deletions
D1
D2
D3
D4
B
Disorder
TM0160 Fragmentation
and peptide deuteration map
TM0160 Truncations
D1
D2
D3
D4
C
TM0160 Full length
TM0160 Deletion D3

Figure 7

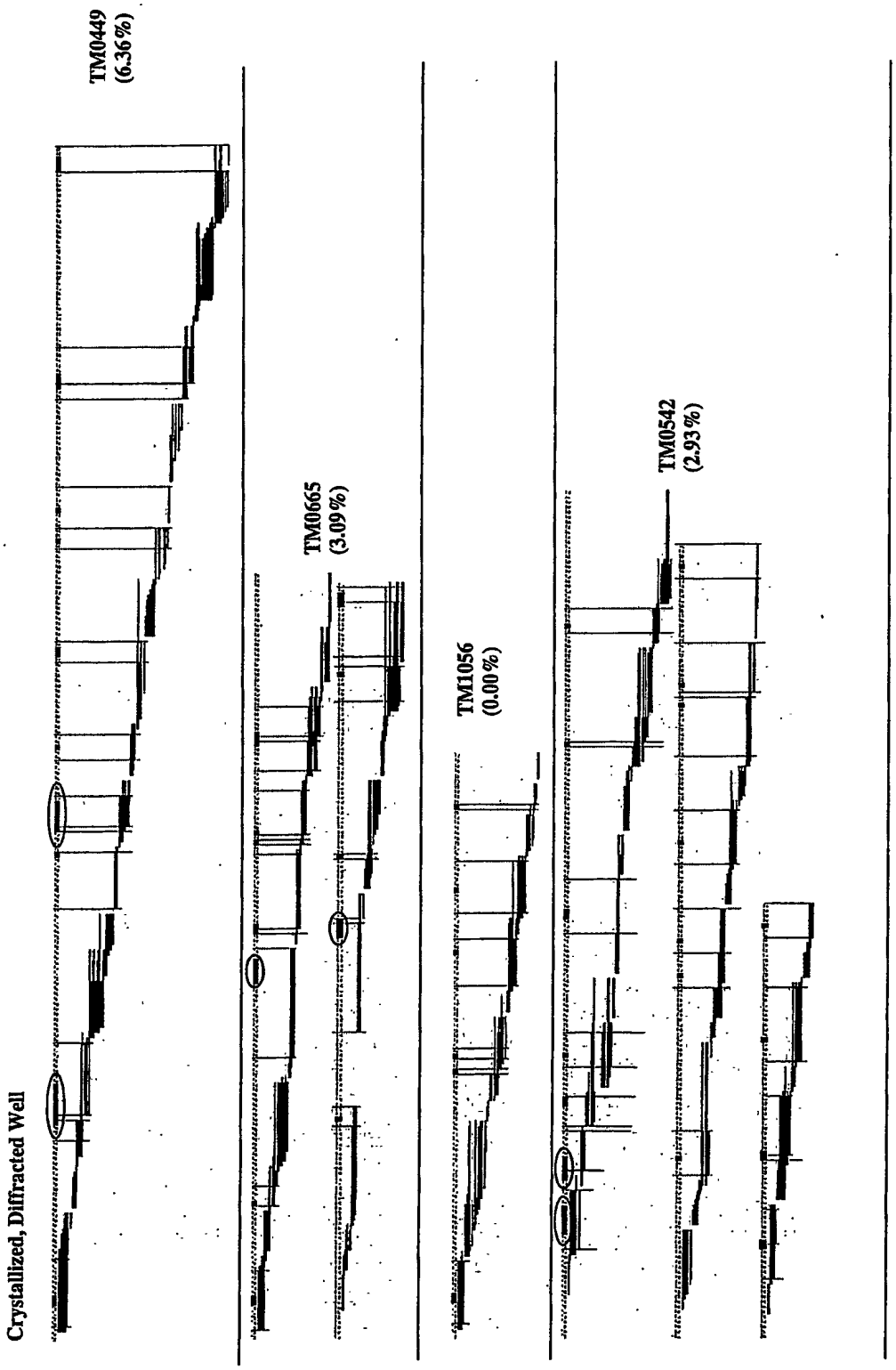
Crystallized, Diffracted Well
TM0449
(6.36%)
TM0665
(3.09%)
TM1056
(0.00%)
TM0542
(2.93%)

Figure 8A

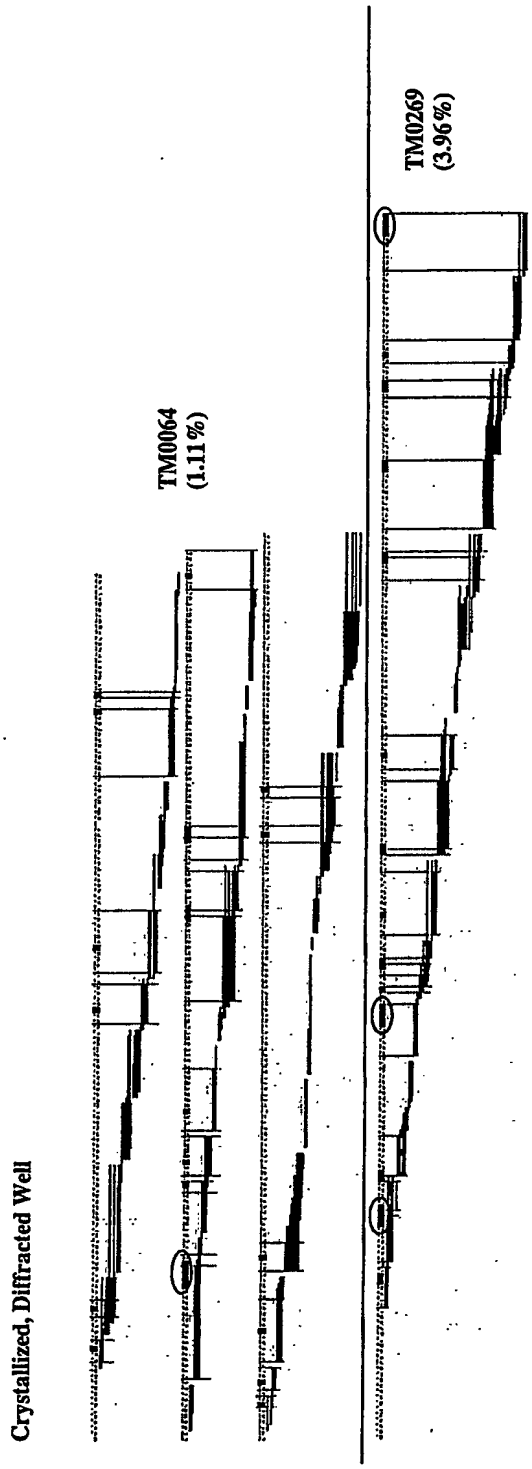

Figure 8B

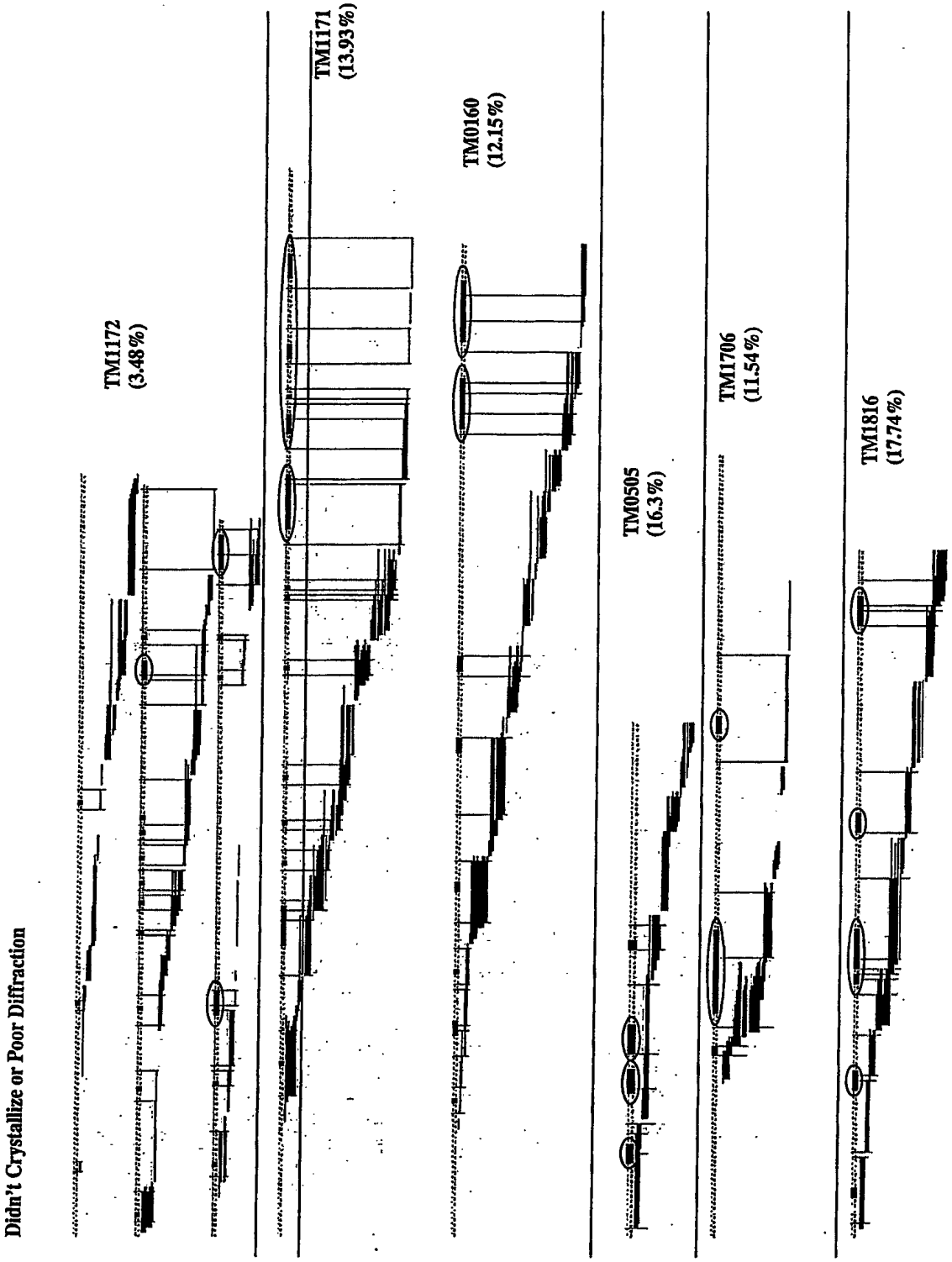
Didn't Crystallize or Poor Diffraction
TM1172
(3.48%)
TM1171
(13.93%)
TM0160
(12.15%)
TM0505
(16.3%)
TM1706
(11.54%)
TM1816
(17.74%)

Figure 8C

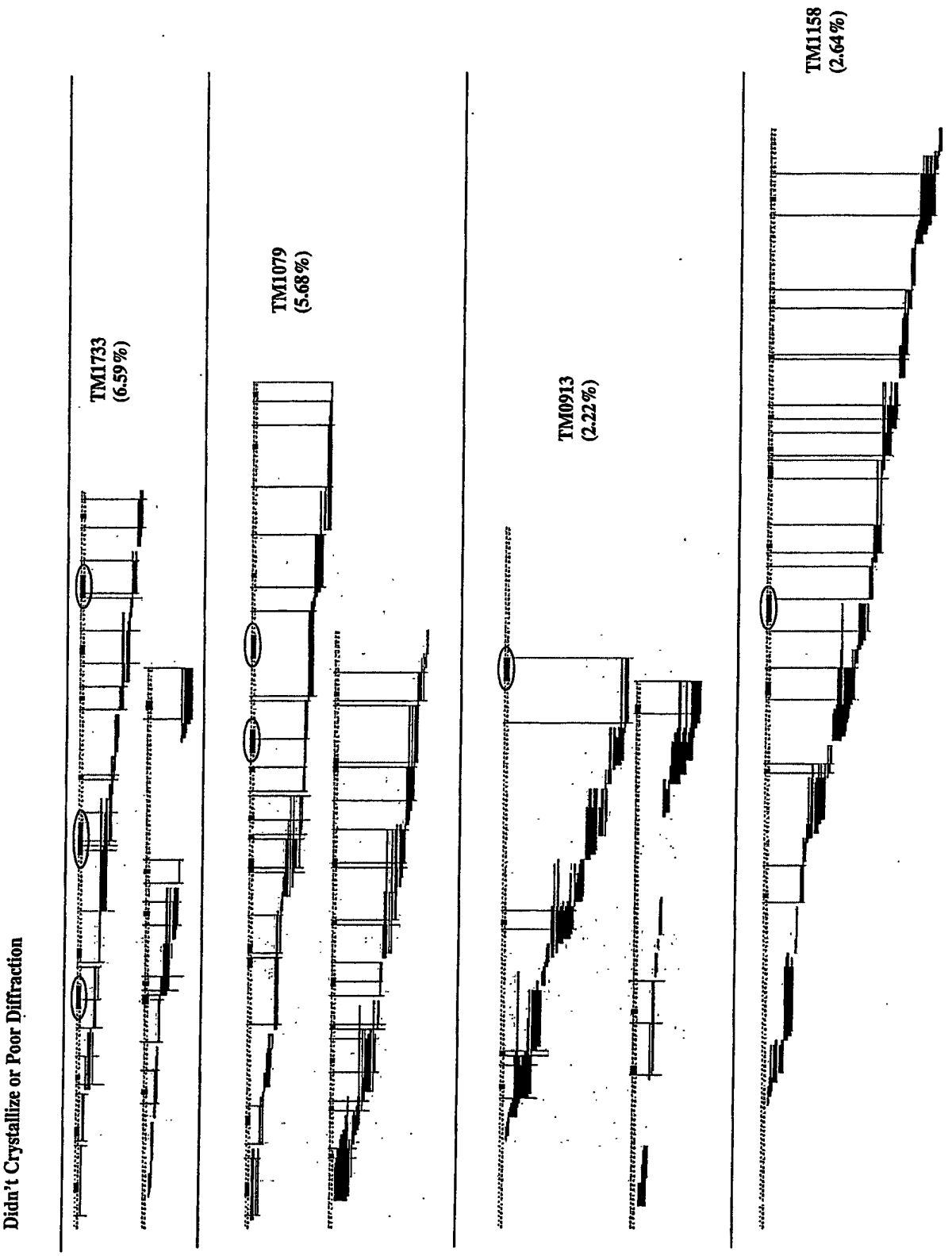
TM1733
(6.59%)
TM1079
(5.68%)
TM0913
(2.22%)
TM1158
(2.64%)
Didn't Crystallize or Poor Diffraction

Figure 8D

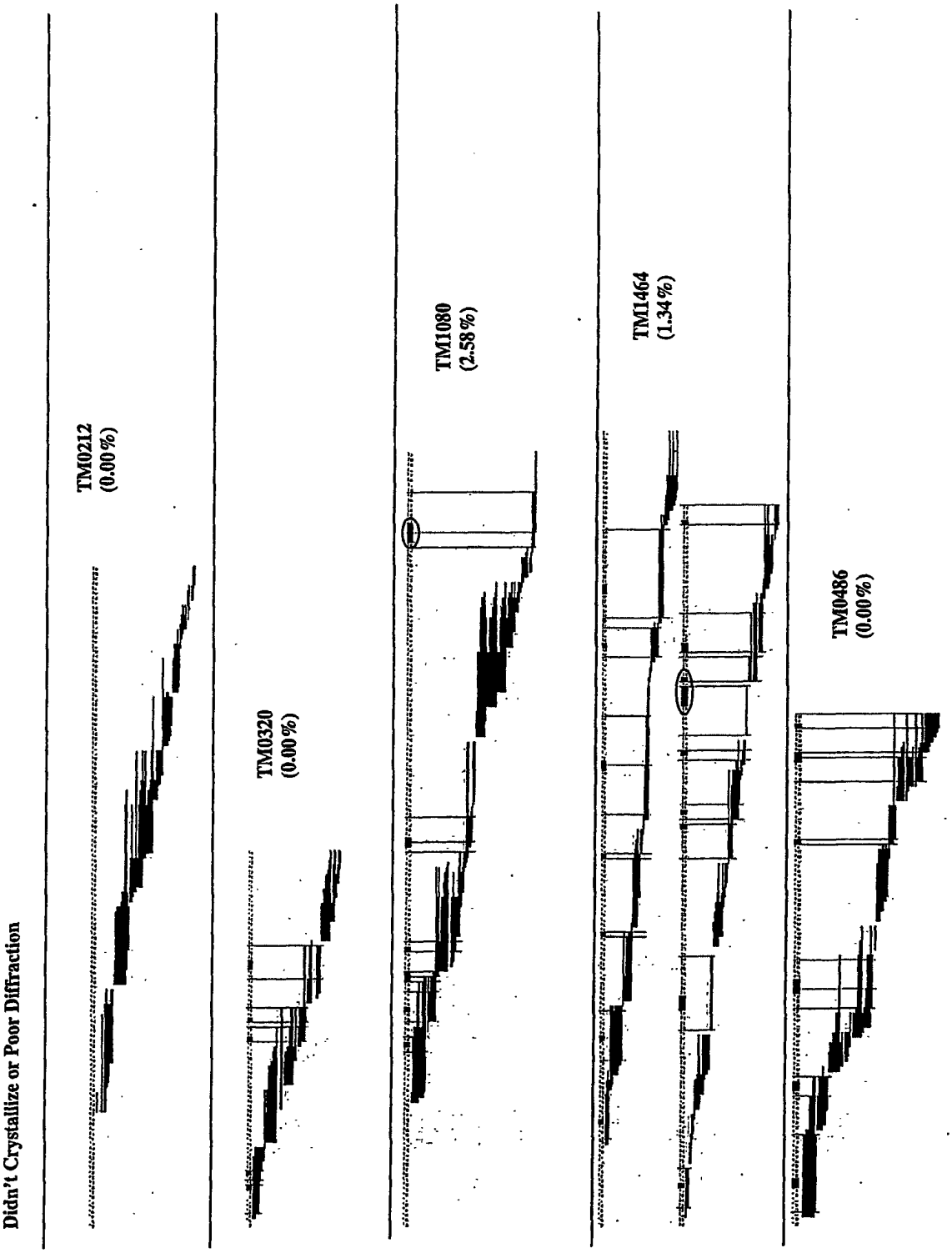
Didn't Crystallize or Poor Diffraction
TM0212
(0.00%)
TM0320
(0.00%)
TM1080
(2.58%)
TM1464
(1.34%)
TM0486
(0.00%)

Figure 8E

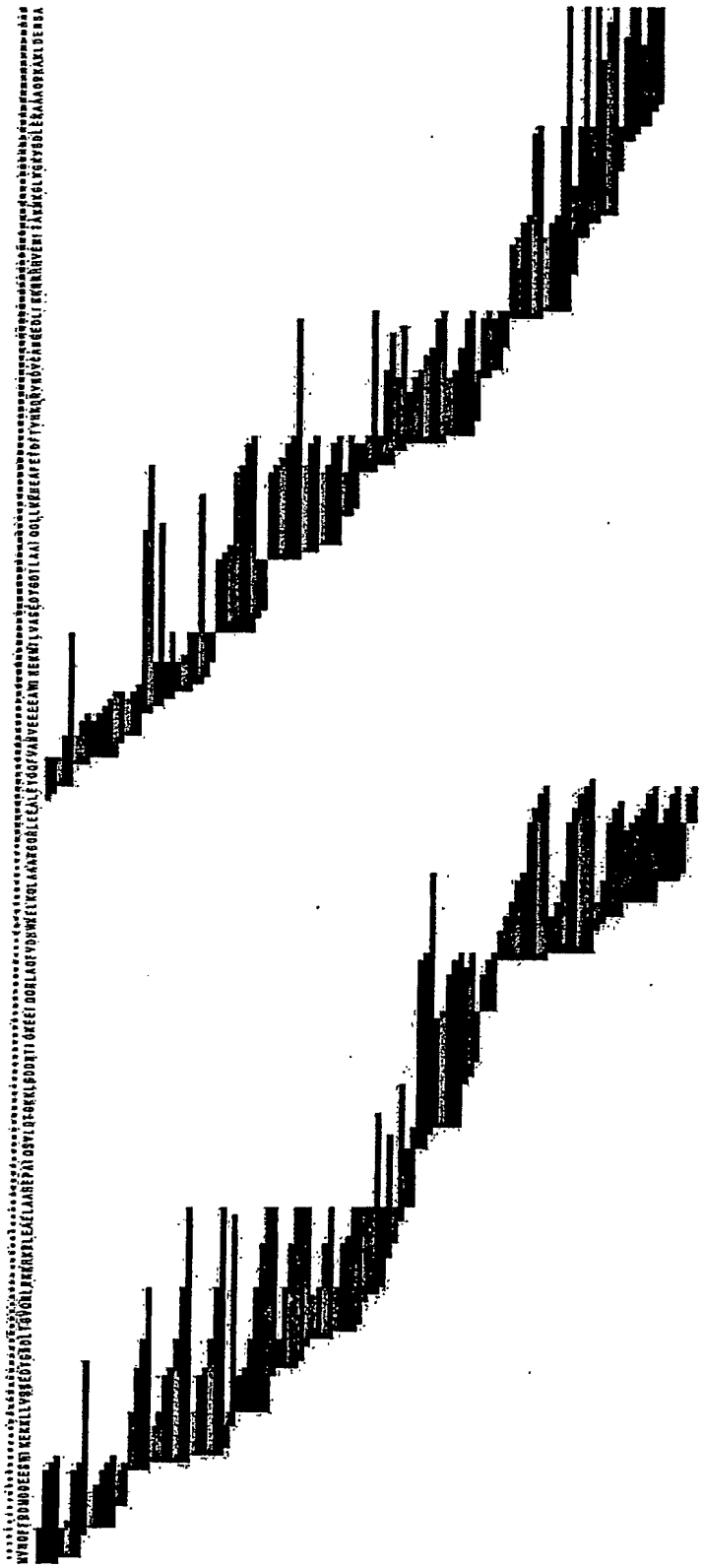

Figure 9

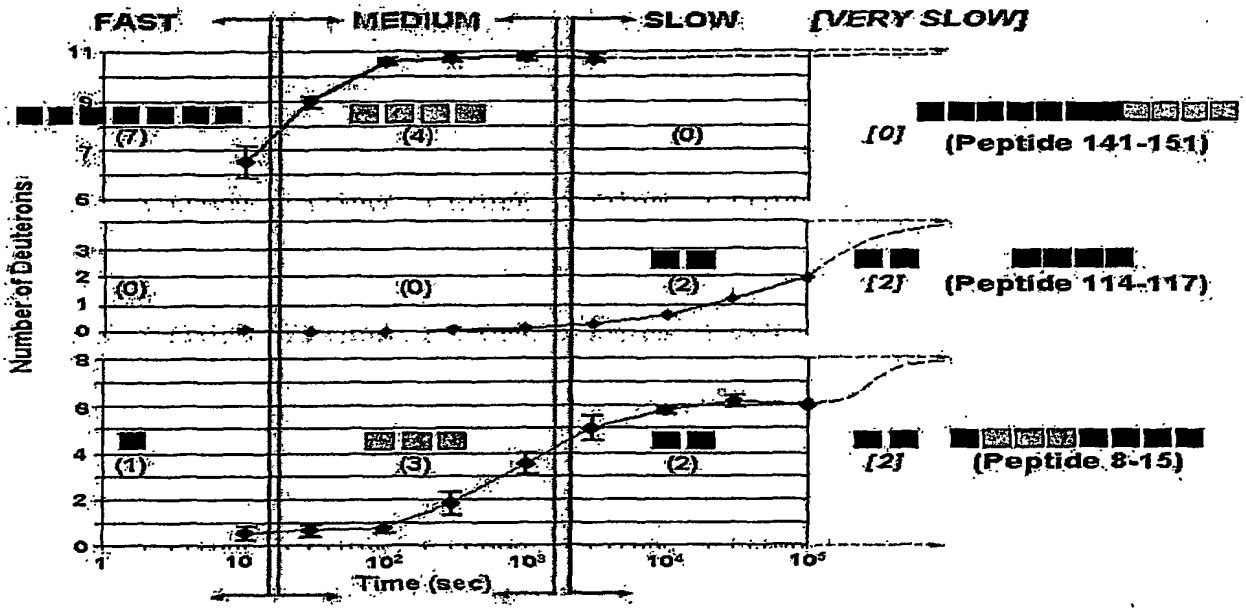
FAST
MEDIUM
SLOW
[VERY SLOW]
Number of Deuterons
Time (sec)
(7)
(4)
(0)
[0]
(Peptide 141-151)
(0)
(0)
(2)
[2]
(Peptide 114-117)
(1)
(3)
(2)
[2]
(Peptide 8-15)

Figure 10

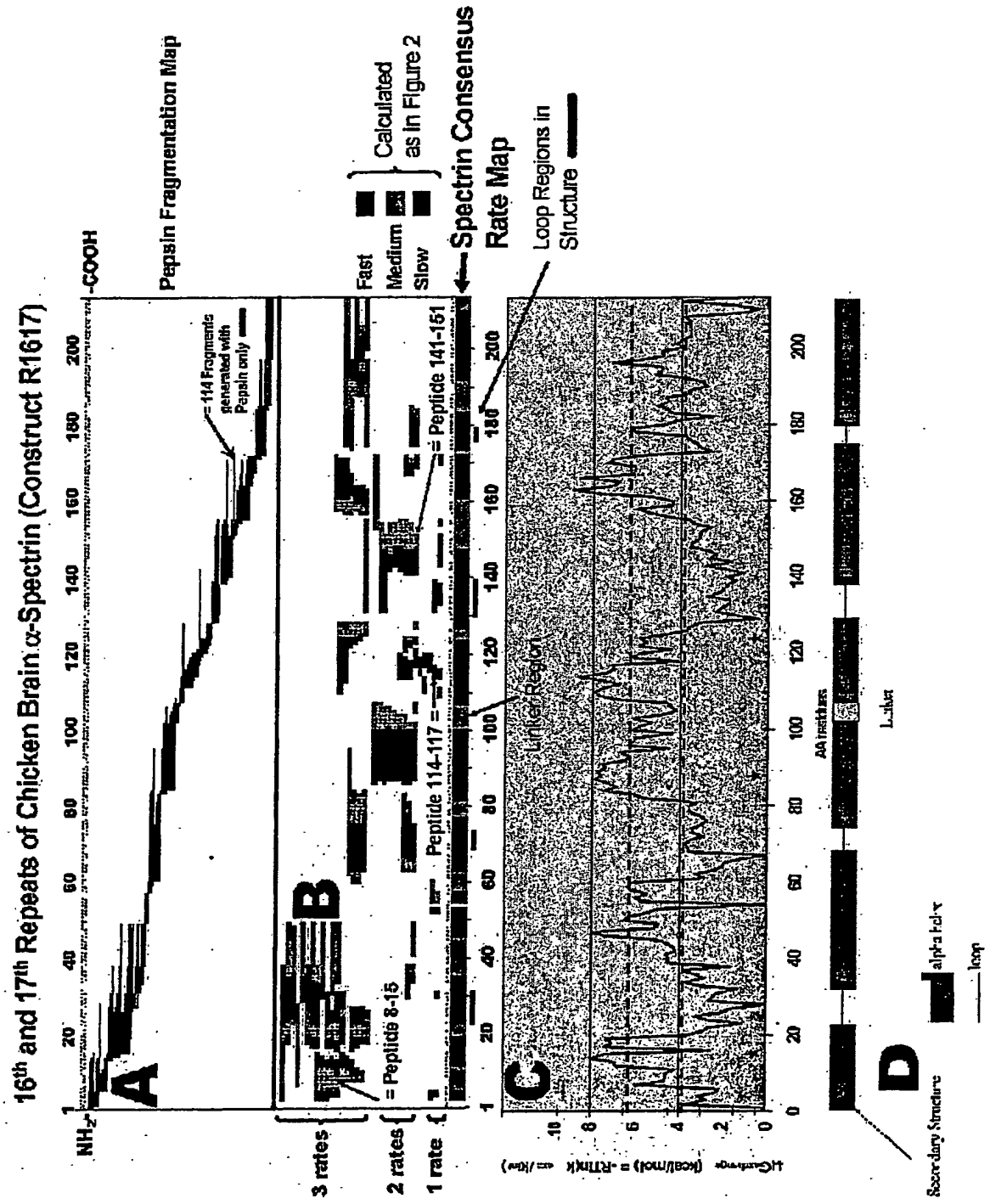
16th and 17th Repeats of Chicken Brain α-Spectrin (Construct R16617)
Pepsin Fragmentation Map
NH2
COOH
A
= 114 Fragments generated with Pepsin only
B
Fast
Medium
Slow
Calculated as in Figure 2
Spectrin Consensus Rate Map
Loop Regions in Structure
3 rates
2 rates
1 rate
= Peptide 8-15
Peptide 114-117 =
= Peptide 141-151
C
Linker Region
AA residues
Linker
D
Secondary Structure
alpha helix
loop

Figure 11

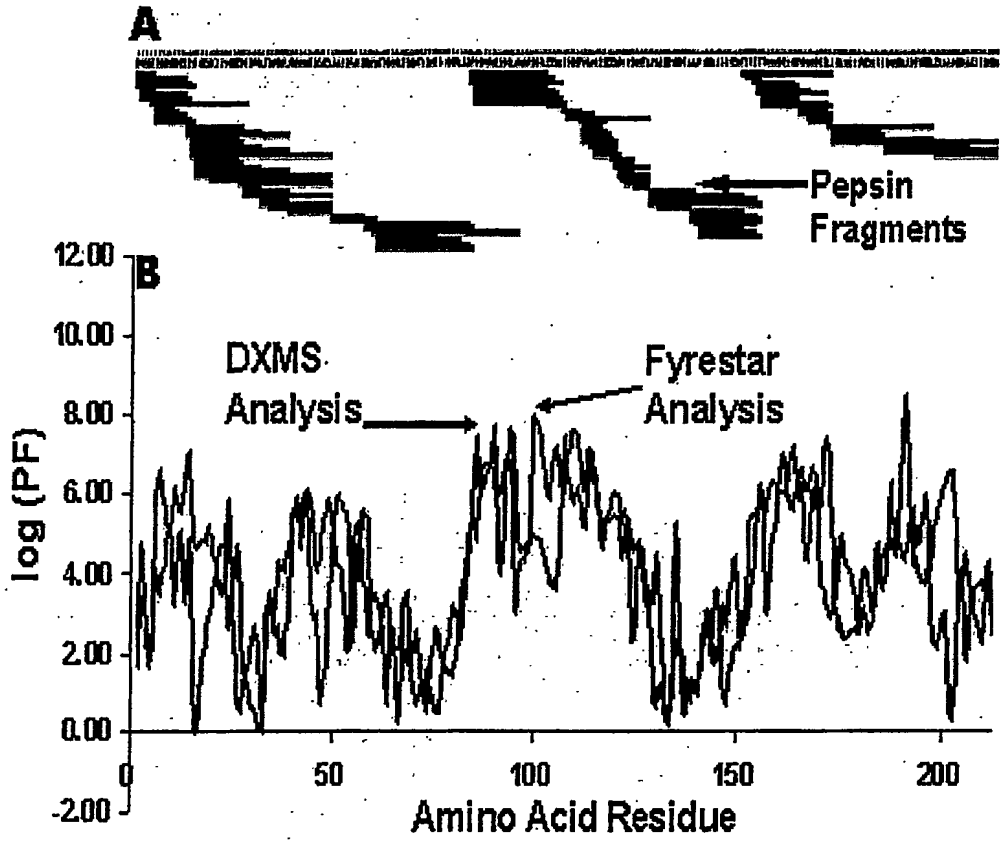
A
Pepsin
Fragments
B
DXMS
Analysis
Fyrestar
Analysis
log (PF)
12.00
10.00
8.00
6.00
4.00
2.00
0.00
-2.00
0
50
100
150
200
Amino Acid Residue

Figure 12

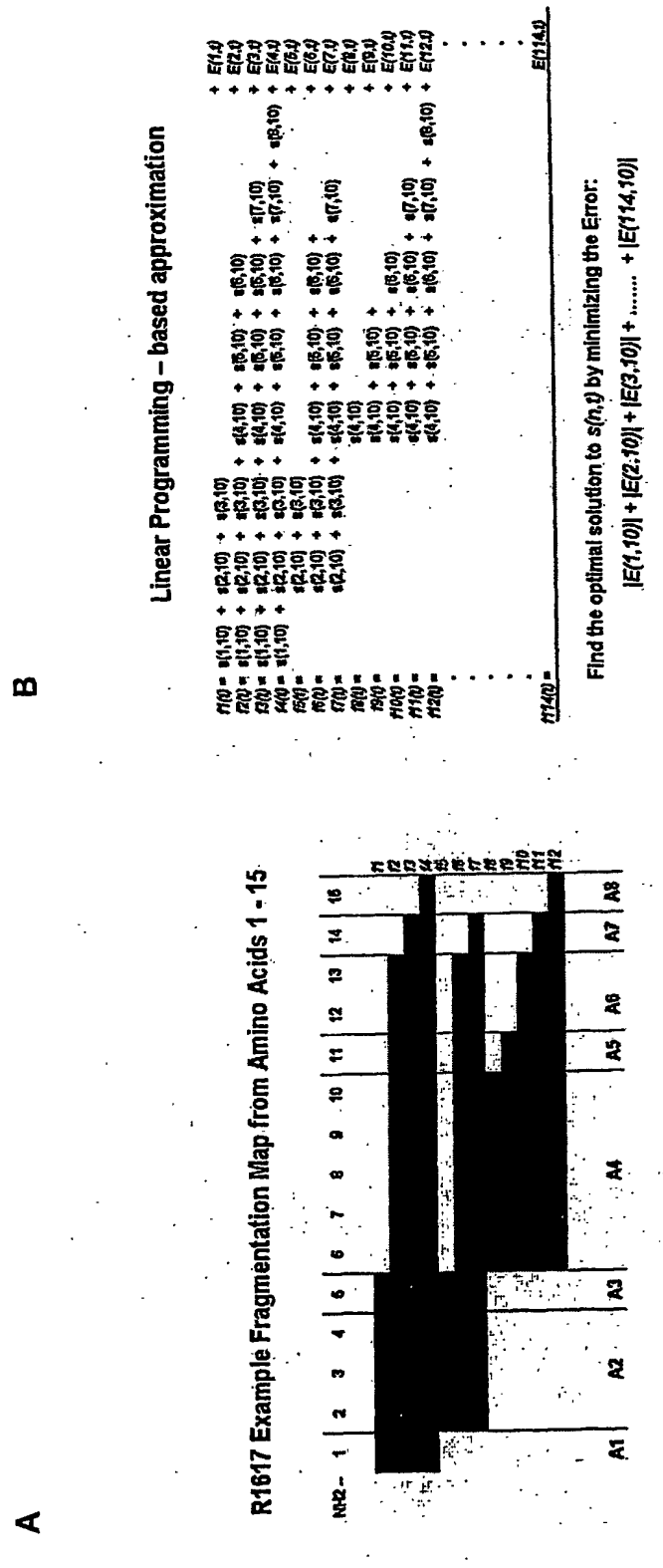
A
R1617 Example Fragmentation Map from Amino Acids 1 - 15
NH2-
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
A1
A2
A3
A4
A5
A6
A7
A8
B
Linear Programming – based approximation
Find the optimal solution to s(n,t) by minimizing the Error:
|E(1,10)| + |E(2,10)| + |E(3,10)| + ... + |E(114,10)|

Figure 13

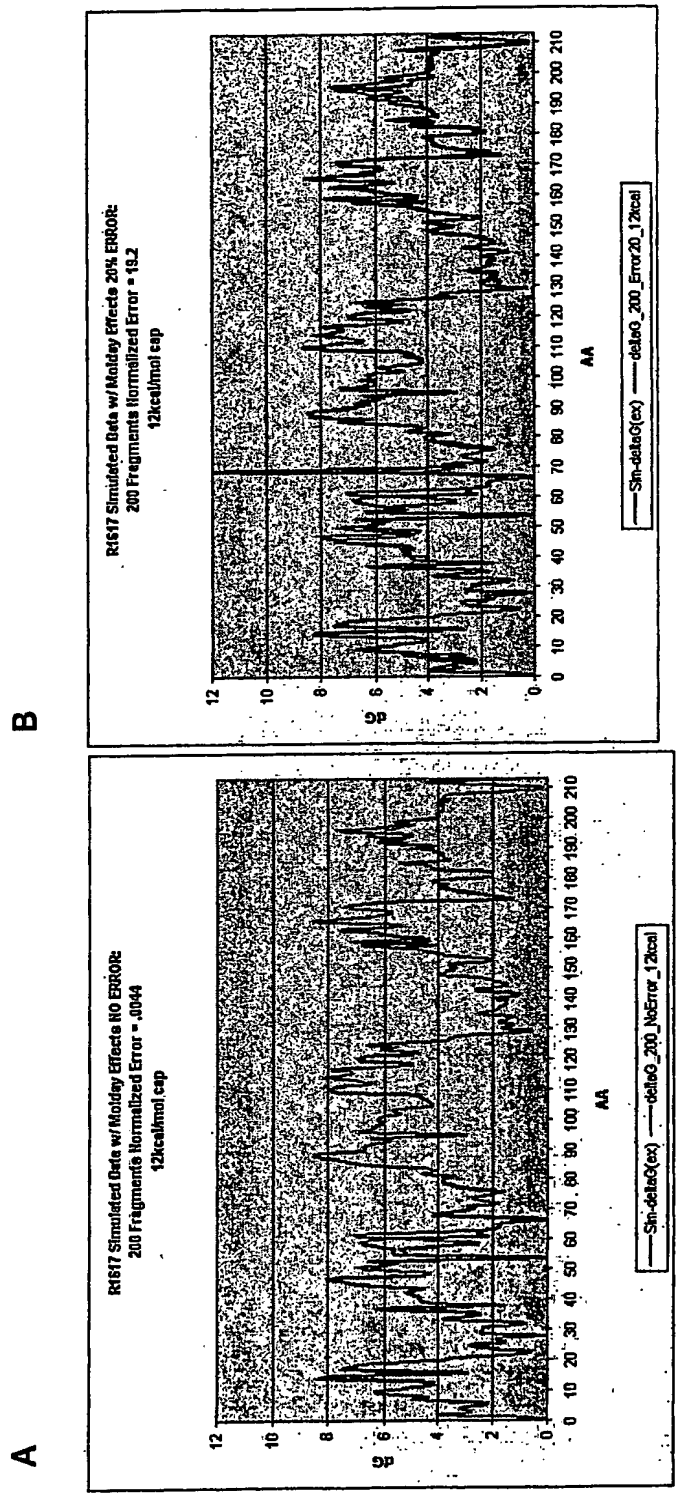
A
R1617 Simulated Data w/ Moldey Effects NO ERROR
200 Fragments Normalized Error = .0044
12kcal/mol cap
dG
AA
Sin-deltaG(ex)
deltaG_200_NoError_12kcal
B
R1617 Simulated Data w/ Moldey Effects 20% ERROR
200 Fragments Normalized Error = 19.2
12kcal/mol cap
dG
AA
Sin-deltaG(ex)
deltaG_200_Error20_12kcal

Figure 14

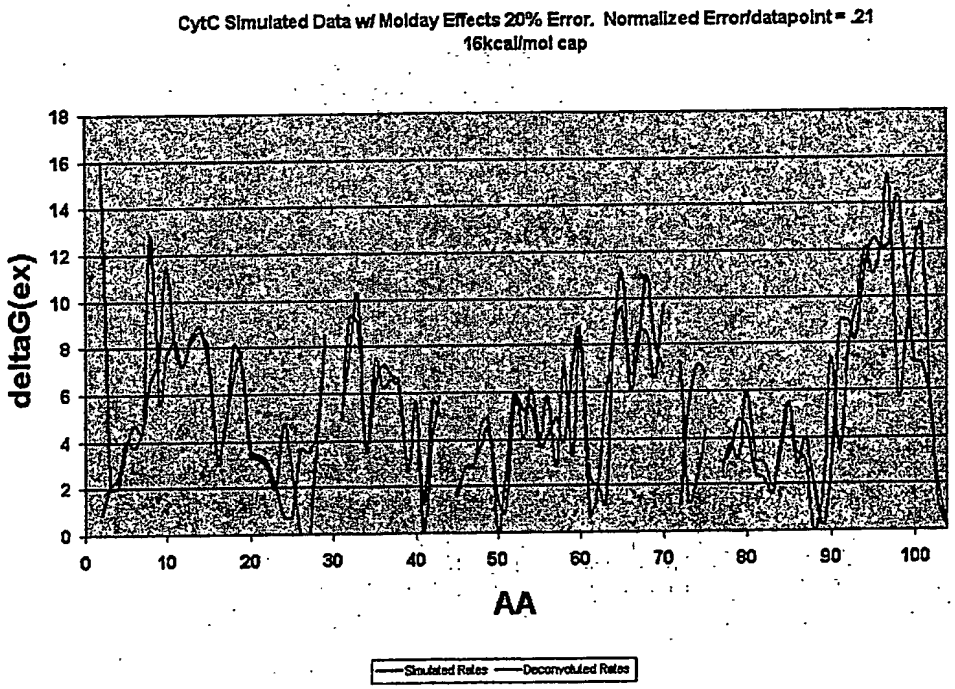
CytC Simulated Data w/ Molday Effects 20% Error. Normalized Error/datapoint = .21
16kcal/mol cap
deltaG(ex)
AA
0
2
4
6
8
10
12
14
16
18
0
10
20
30
40
50
60
70
80
90
100
Simulated Rates
Deconvoluted Rates

Figure 15

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